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Evaluating New Double Perovskite Halide Scintillators for Radiation Detection Applications

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Materials Science and Technology (MST) Division

MST-8 Materials Science in Radiation and Dynamics Extremes

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LA-UR-XXXXXX

Summer Activities

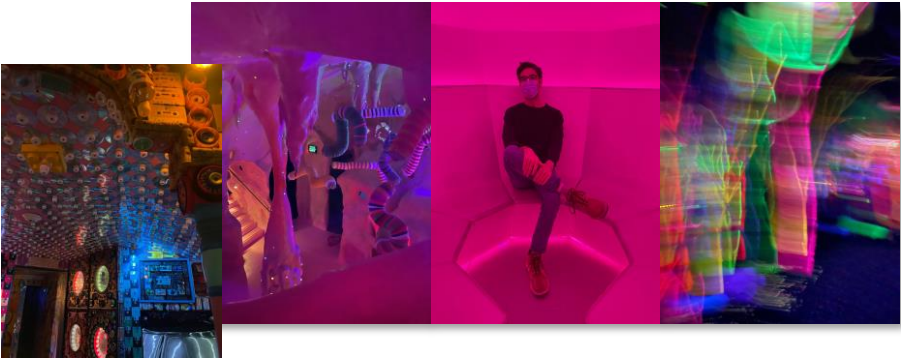


White Rock Overlook



Tsankawi Trail (Los Alamos)

Meow Wolf (Santa Fe)



Daniel Rutstrom (MST-8)

- Educational Background

- B.S. in MSE, University of Tennessee, 2018
- M.S. in MSE, University of Tennessee, 2021

- Division

- Materials Science in Radiation and Dynamics Extremes (MST-8)
- Mentor: Ken McClellan

- Research

- Experimental validation of machine learning based scintillator prediction models
- Discovery and development of advanced halide scintillators for gamma spectroscopy applications



THE UNIVERSITY OF
TENNESSEE
KNOXVILLE

Daniel Rutstrom



Ken McClellan

Research Overview and Motivation

- **Objectives**

- Provide experimental data to feed back in to models for high-throughput predictions of potential new scintillator materials
- Identify promising scintillator compounds to pursue further

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- Provide experimental data to feed back in to models for high-throughput predictions of potential new scintillator materials
- Identify promising scintillator compounds to pursue further

- **Motivation:**

- **Ideal scintillator does not exist, new materials with tailored properties are desired**
- Discovery of new scintillator compounds can be lengthy and tedious
- Complimentary use of modeling and experimental work can provide a more efficient approach than conventional “trial and error” approach
 - **Rapid screening, vast chemical spaces**

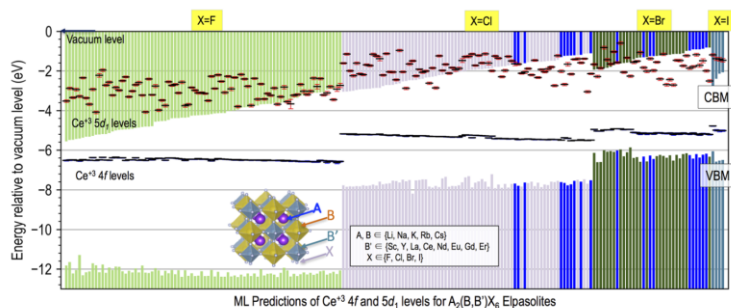
- **Applications:** gamma spectroscopy, flash radiography, etc.

Research Approach

Fabrication of predicted new scintillators

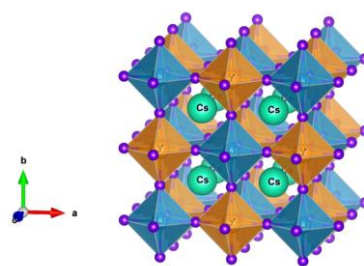
- Selected a set of new compounds to pursue experimentally, based on calculated electronic band structures
- Compositional space – double perovskite halides \longrightarrow $A_2BB'X_6:Ce$ ($A = Rb^+, Cs^+$; $B = Na^+, K^+$; $B' = RE^{3+}$; $X = Cl^-, Br^-$)
- Fabrication method – single crystal growth via Bridgman technique
- Characterization – physical, optical, and scintillation properties

Positions of Ce^{3+} 5d and 4f energy levels relative to CB and VB for 200 Double Perovskite Halides

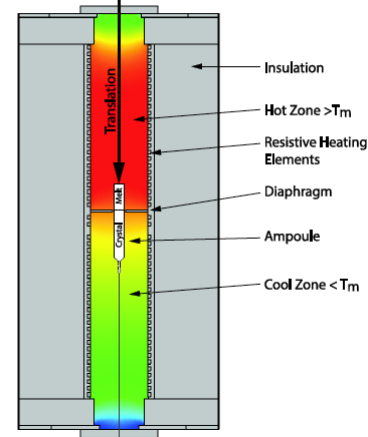


G. Pilania *et al.* "Physics-informed machine learning for inorganic scintillator discovery" J. Chem. Phys. **148**, 241729 (2018)

Double perovskite structural model (Cs_2LiYCl_6)



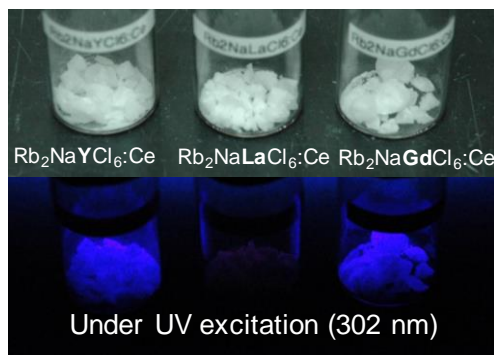
Bridgman Method



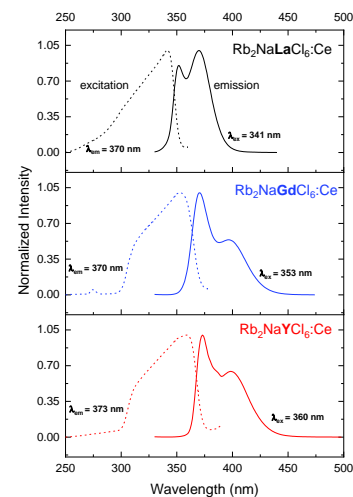
Summary of Results

- **Synthesized 3 new compounds**
 - $\text{Rb}_2\text{NaYCl}_6:\text{Ce}$
 - $\text{Rb}_2\text{NaLaCl}_6:\text{Ce}$
 - $\text{Rb}_2\text{NaGdCl}_6:\text{Ce}$
- **All three compositions luminesce**
- **$\text{Rb}_2\text{NaGdCl}_6:\text{Ce}$ is most promising, highest intensity emission**
- **Determined melting points via DSC**
(not reported in literature since these are new materials)
- **In progress**
 - Crystal growth
 - X-ray diffraction

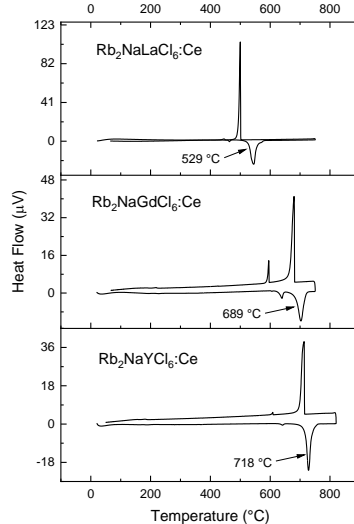
Synthesized polycrystalline samples



Photoluminescence



Differential Scanning Calorimetry (DSC)



Radioluminescence (X-ray) Emission Spectra

